



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:43 am BST

PDB ID : 3BNY
Title : Crystal structure of aristolochene synthase complexed with 2-fluorofarnesyl diphosphate (2F-FPP)
Authors : Shishova, E.Y.; Christianson, D.W.
Deposited on : 2007-12-14
Resolution : 1.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

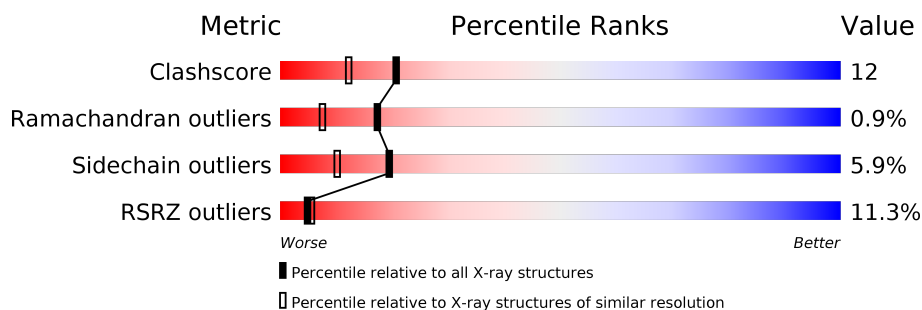
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	320	<div> <div>9%</div> <div>76%</div> <div>14%</div> <div>• 8%</div> </div>
1	B	320	<div> <div>10%</div> <div>68%</div> <div>21%</div> <div>• 8%</div> </div>
1	C	320	<div> <div>12%</div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div>
1	D	320	<div> <div>10%</div> <div>69%</div> <div>20%</div> <div>• • 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FPF	C	402	-	-	X	-
4	BME	C	1270	-	-	X	-

2 Entry composition [i](#)

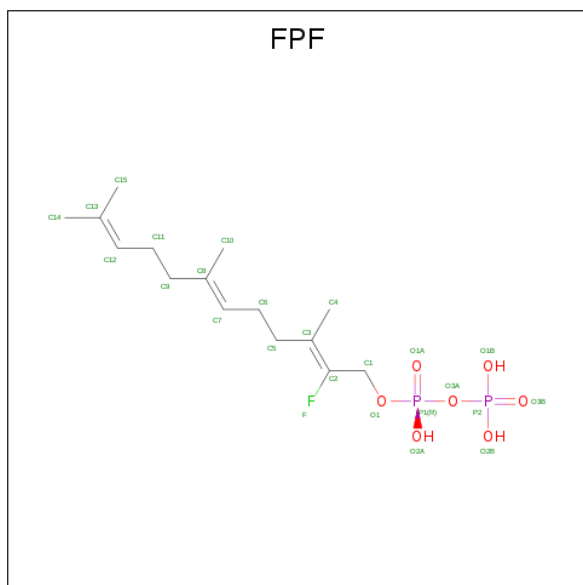
There are 6 unique types of molecules in this entry. The entry contains 10204 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2385	1525	402	443	15			
1	B	296	Total	C	N	O	S	0	0	0
			2400	1535	404	446	15			
1	C	293	Total	C	N	O	S	0	0	0
			2375	1518	401	441	15			
1	D	297	Total	C	N	O	S	0	0	0
			2407	1538	406	448	15			

- Molecule 2 is (2Z,6E)-2-fluoro-3,7,11-trimethyldodeca-2,6,10-trien-1-yl trihydrogen diphosphate (three-letter code: FPF) (formula: C₁₅H₂₇FO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	P	0	0
			25	15	1	7	2		
2	B	1	Total	C	F	O	P	0	0
			25	15	1	7	2		

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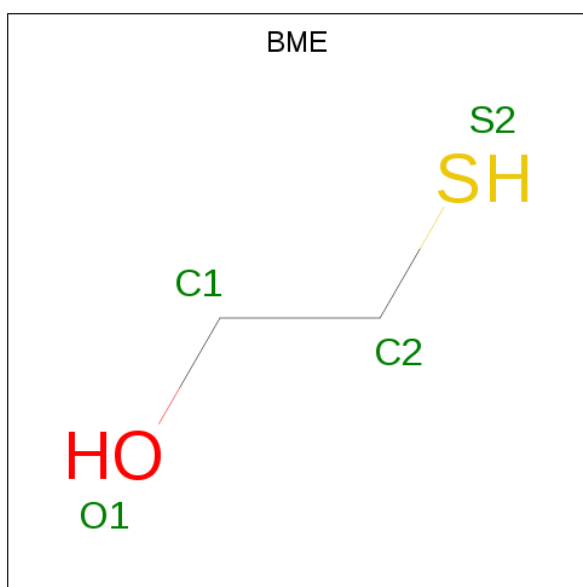
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	O	P	0	0
			25	15	1	7	2		
2	D	1	Total	C	F	O	P	0	0
			25	15	1	7	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



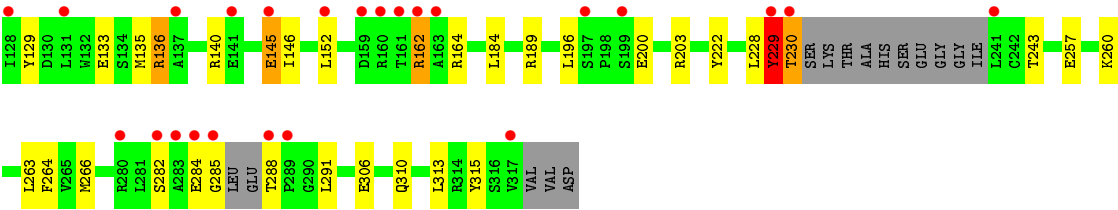
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

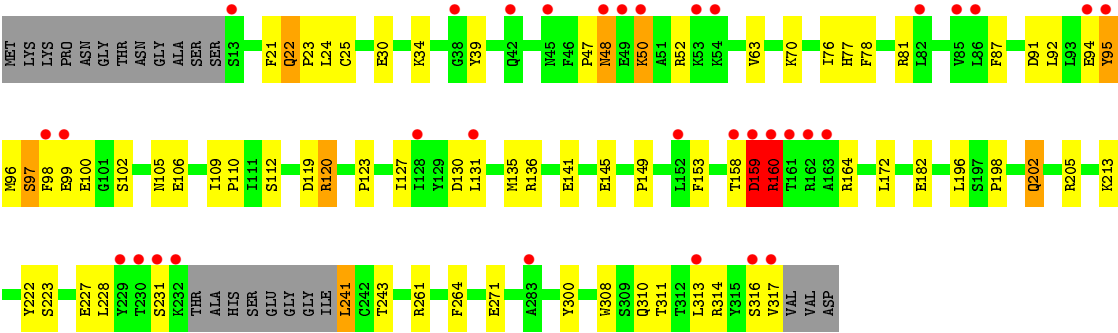
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0
6	B	116	Total 116	O 116	0	0
6	C	122	Total 122	O 122	0	0
6	D	150	Total 150	O 150	0	0



● Molecule 1: Aristolochene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.65Å 147.86Å 83.95Å 90.00° 97.84° 90.00°	Depositor
Resolution (Å)	22.33 – 1.89 22.33 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (22.33-1.89) 88.8 (22.33-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.264 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10204	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FPF, CL, BME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/2438	0.65	0/3299
1	B	0.52	0/2453	0.65	1/3320 (0.0%)
1	C	0.55	0/2427	0.65	0/3283
1	D	0.56	0/2460	0.71	3/3328 (0.1%)
All	All	0.54	0/9778	0.67	4/13230 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	ASP	CA-C-N	-6.36	103.22	117.20
1	D	159	ASP	C-N-CA	5.66	135.85	121.70
1	B	316	SER	CA-C-N	-5.63	104.82	117.20
1	D	160	ARG	CA-C-N	-5.32	105.50	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2385	0	2358	38	0
1	B	2400	0	2376	80	0
1	C	2375	0	2346	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2407	0	2382	59	0
2	A	25	0	24	6	0
2	B	25	0	24	8	0
2	C	25	0	24	9	0
2	D	25	0	22	6	0
3	B	1	0	0	0	0
4	B	4	0	6	2	0
4	C	4	0	5	4	0
4	D	4	0	5	1	0
5	D	1	0	0	0	0
6	A	135	0	0	3	0
6	B	116	0	0	2	0
6	C	122	0	0	0	0
6	D	150	0	0	2	0
All	All	10204	0	9572	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 237 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:CYS:SG	4:C:1270:BME:S2	2.29	1.30
1:D:25:CYS:SG	4:D:1272:BME:S2	2.32	1.25
2:C:402:FPP:H1A	2:C:402:FPP:O3B	1.47	1.14
1:C:66:LEU:HG	4:C:1270:BME:H12	1.26	1.13
1:B:52:ARG:HH11	1:B:52:ARG:HG3	1.01	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/320 (91%)	285 (98%)	5 (2%)	0	100	100
1	B	292/320 (91%)	281 (96%)	7 (2%)	4 (1%)	11	3
1	C	287/320 (90%)	273 (95%)	12 (4%)	2 (1%)	22	12
1	D	293/320 (92%)	283 (97%)	5 (2%)	5 (2%)	9	2
All	All	1162/1280 (91%)	1122 (97%)	29 (2%)	11 (1%)	17	7

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	PRO
1	C	229	TYR
1	D	97	SER
1	D	47	PRO
1	D	159	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/279 (93%)	247 (95%)	12 (5%)	27	17
1	B	261/279 (94%)	243 (93%)	18 (7%)	15	7
1	C	258/279 (92%)	245 (95%)	13 (5%)	24	15
1	D	262/279 (94%)	244 (93%)	18 (7%)	15	7
All	All	1040/1116 (93%)	979 (94%)	61 (6%)	19	10

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	264	PHE
1	C	145	GLU
1	D	196	LEU
1	B	313	LEU
1	C	22	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	219	ASN
1	B	305	ASN
1	D	48	ASN
1	B	77	HIS
1	B	105	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FPF	D	403	5	22,24,24	5.15	10 (45%)	24,33,33	3.72	9 (37%)
4	BME	B	1271	-	3,3,3	0.23	0	1,2,2	0.73	0
4	BME	D	1272	-	3,3,3	0.33	0	1,2,2	0.40	0
4	BME	C	1270	-	3,3,3	0.27	0	1,2,2	0.54	0
2	FPF	A	400	-	22,24,24	2.40	3 (13%)	24,33,33	2.87	9 (37%)
2	FPF	B	401	-	22,24,24	10.84	3 (13%)	24,33,33	2.15	7 (29%)
2	FPF	C	402	-	22,24,24	4.93	3 (13%)	24,33,33	2.15	7 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FPF	D	403	5	-	8/22/28/28	-
4	BME	B	1271	-	-	0/1/1/1	-
4	BME	D	1272	-	-	0/1/1/1	-
4	BME	C	1270	-	-	0/1/1/1	-
2	FPF	A	400	-	-	3/22/28/28	-
2	FPF	B	401	-	-	5/22/28/28	-
2	FPF	C	402	-	-	1/22/28/28	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FPF	O1-C1	-50.17	1.08	1.43
2	C	402	FPF	O1-C1	21.64	1.58	1.43
2	D	403	FPF	C4-C3	-13.47	1.28	1.50
2	D	403	FPF	C3-C2	10.88	1.45	1.32
2	A	400	FPF	F-C2	-9.56	1.24	1.36

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	FPF	C5-C6-C7	9.12	141.85	111.88
2	D	403	FPF	C15-C13-C14	8.54	133.47	114.60
2	D	403	FPF	P1-O3A-P2	-7.61	106.72	132.83
2	B	401	FPF	P1-O3A-P2	-7.60	106.75	132.83
2	A	400	FPF	P1-O3A-P2	-7.60	106.75	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

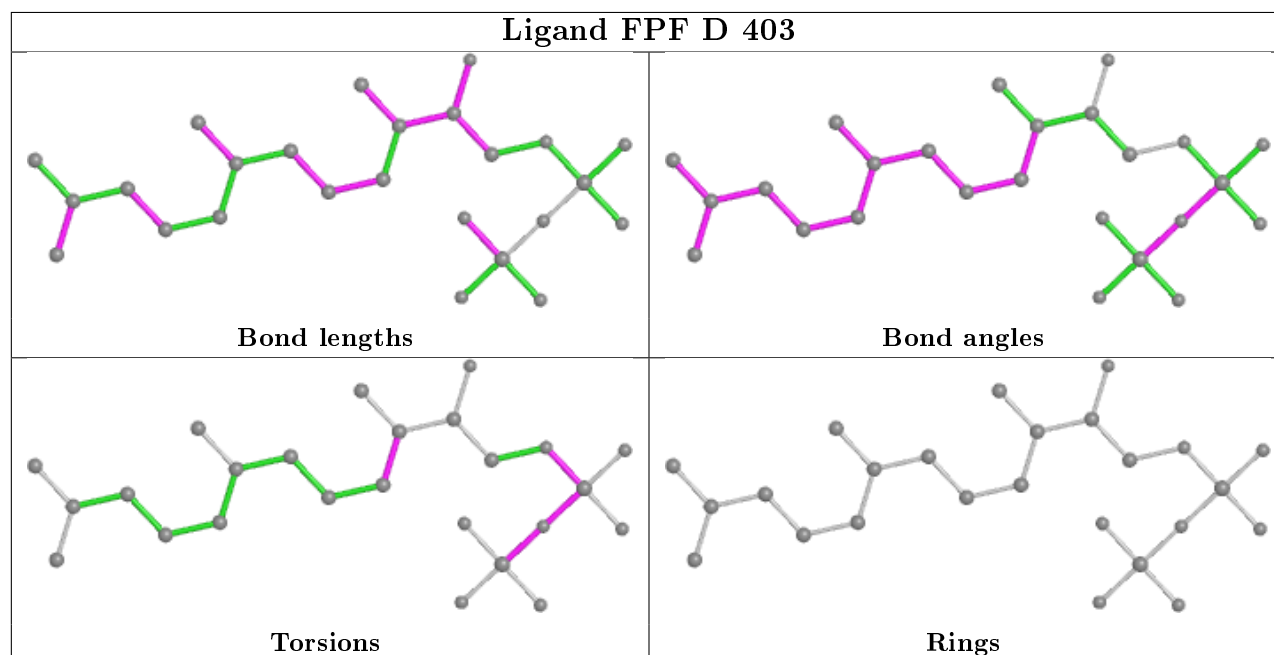
Mol	Chain	Res	Type	Atoms
2	D	403	FPF	C1-O1-P1-O1A
2	D	403	FPF	C2-C3-C5-C6
2	D	403	FPF	P1-O3A-P2-O2B
2	A	400	FPF	C1-O1-P1-O1A
2	B	401	FPF	C1-O1-P1-O3A

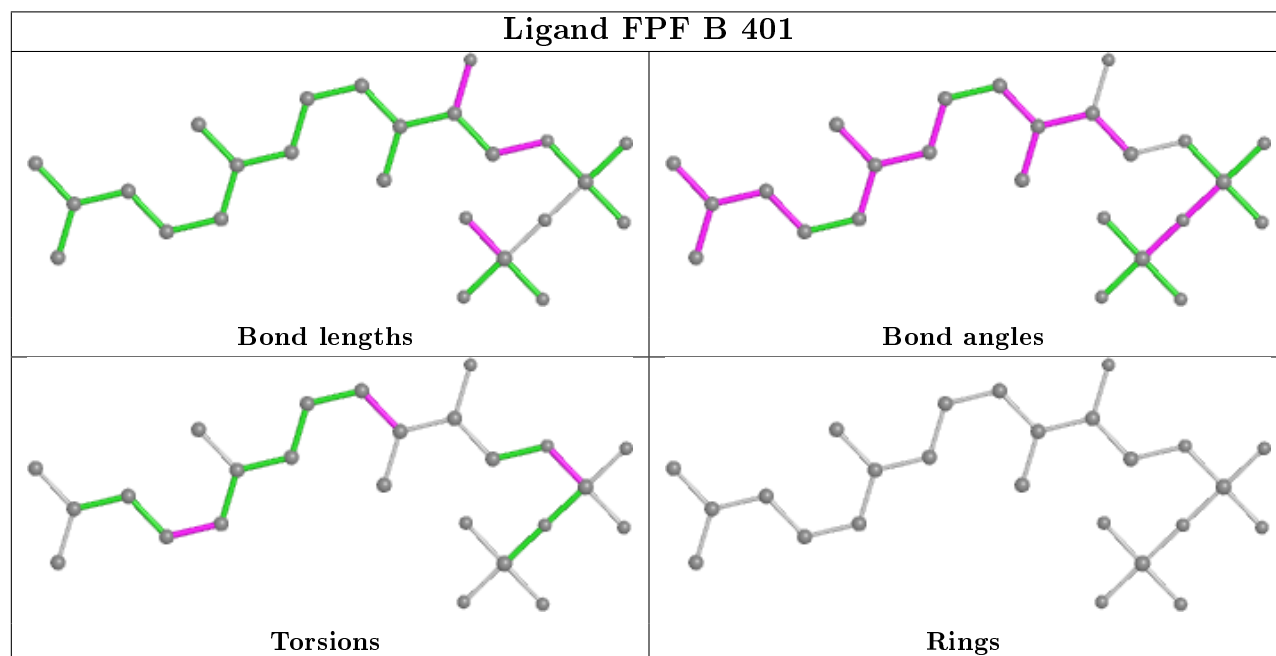
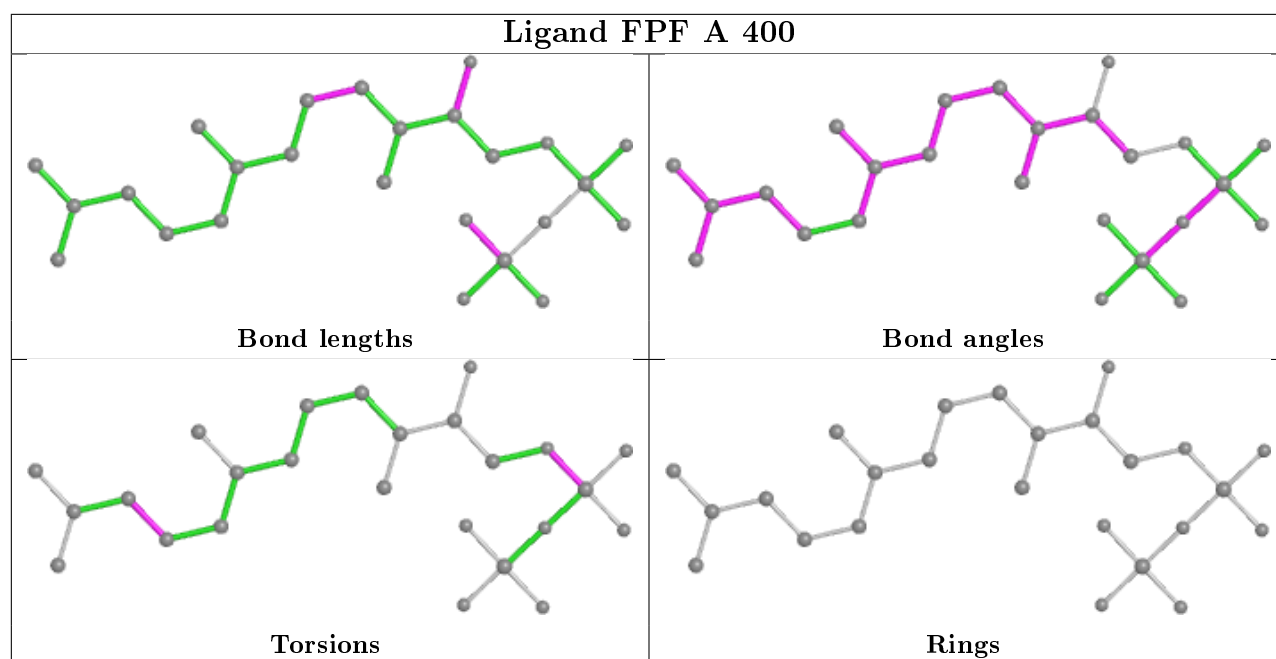
There are no ring outliers.

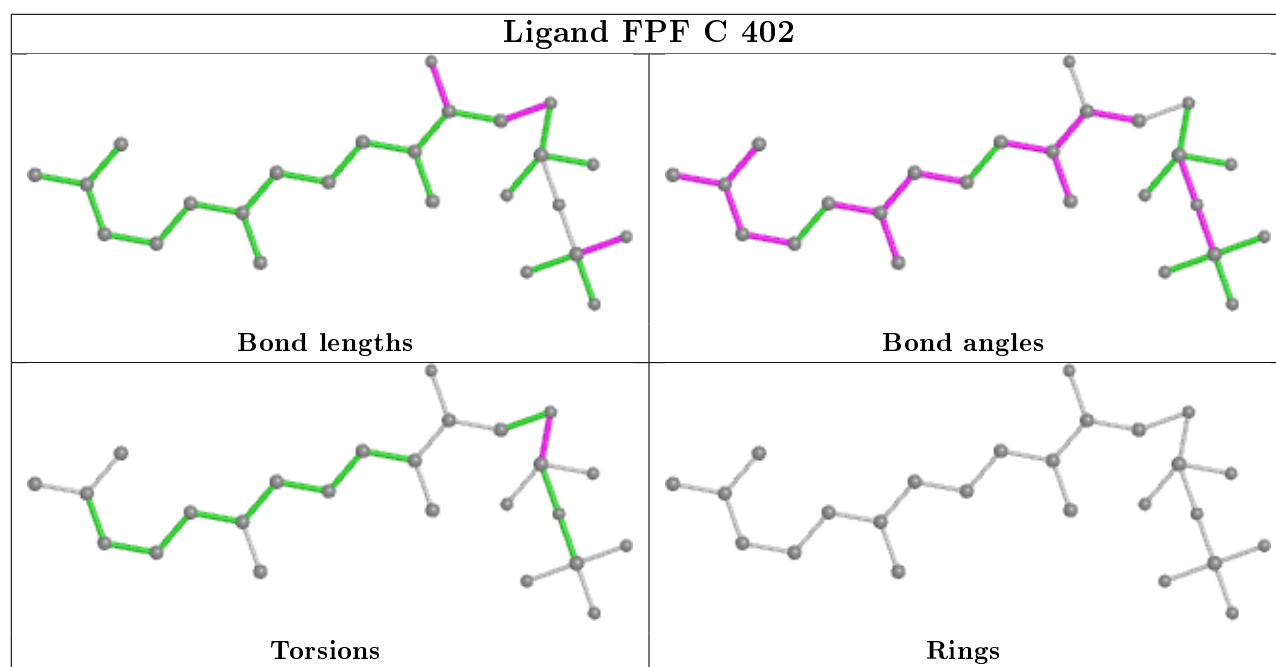
7 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	FPF	6	0
4	B	1271	BME	2	0
4	D	1272	BME	1	0
4	C	1270	BME	4	0
2	A	400	FPF	6	0
2	B	401	FPF	8	0
2	C	402	FPF	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/320 (91%)	0.51	30 (10%) 6 8	14, 27, 51, 63	0
1	B	296/320 (92%)	0.62	33 (11%) 5 6	15, 30, 50, 67	0
1	C	293/320 (91%)	0.61	37 (12%) 3 4	16, 29, 57, 70	0
1	D	297/320 (92%)	0.55	33 (11%) 5 6	12, 26, 58, 72	0
All	All	1180/1280 (92%)	0.58	133 (11%) 5 5	12, 28, 54, 72	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	THR	7.8
1	D	229	TYR	7.7
1	A	98	PHE	6.9
1	D	317	VAL	6.9
1	A	51	ALA	6.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

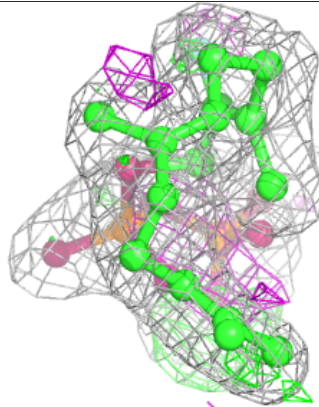
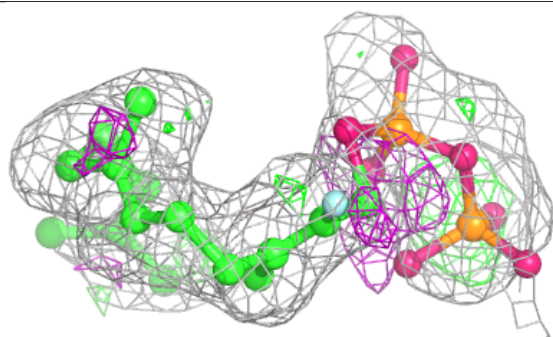
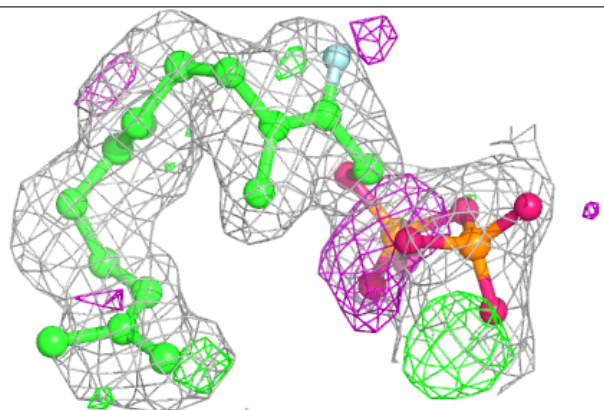
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FPF	C	402	25/25	0.61	0.26	42,48,63,64	0
2	FPF	B	401	25/25	0.69	0.23	45,50,65,65	0
2	FPF	A	400	25/25	0.72	0.23	31,37,58,60	0
4	BME	B	1271	4/4	0.78	0.37	44,44,44,47	4
4	BME	D	1272	4/4	0.82	0.19	30,30,30,36	0
4	BME	C	1270	4/4	0.88	0.15	29,31,33,39	0
2	FPF	D	403	25/25	0.89	0.18	27,38,46,49	0
5	MG	D	701	1/1	0.95	0.05	29,29,29,29	0
3	CL	B	500	1/1	0.96	0.08	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

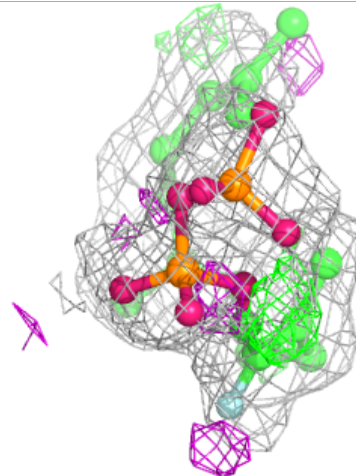
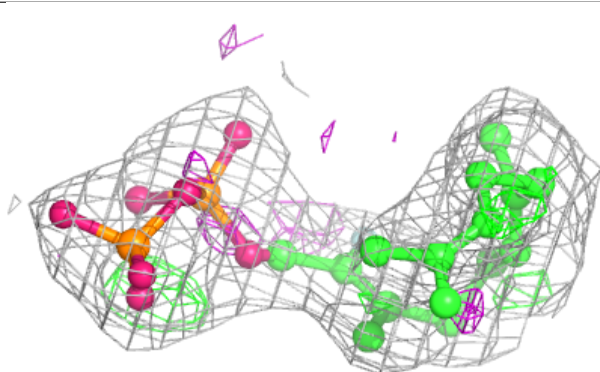
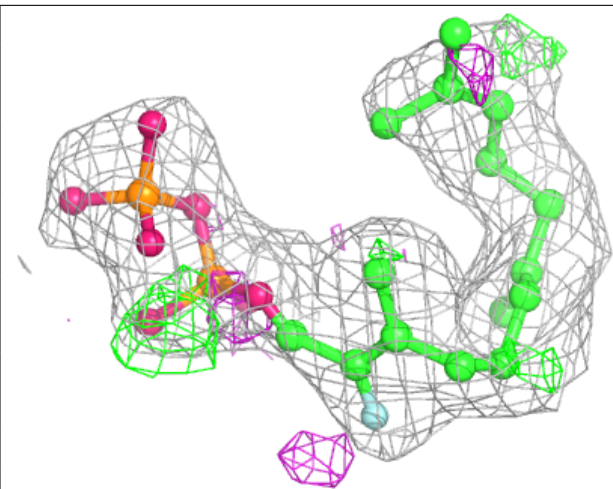
Electron density around FPF C 402:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



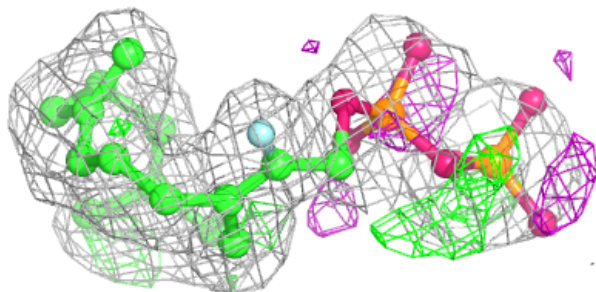
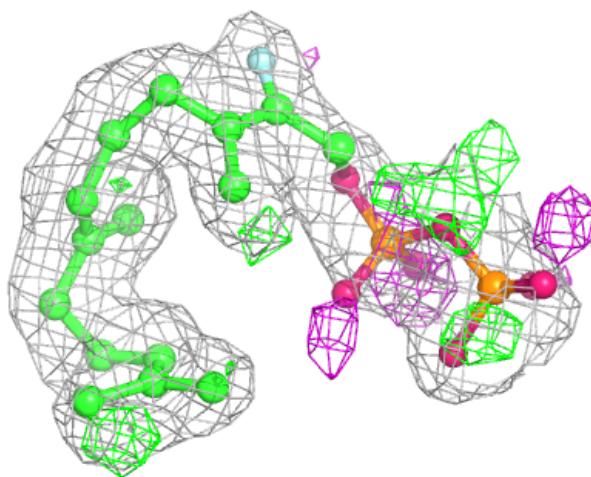
Electron density around FPF B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



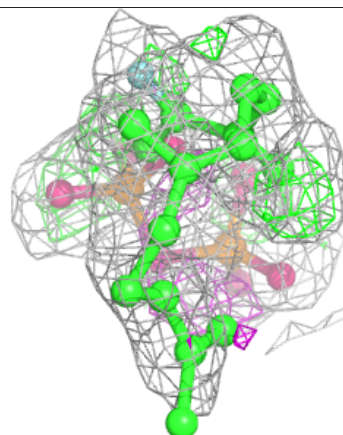
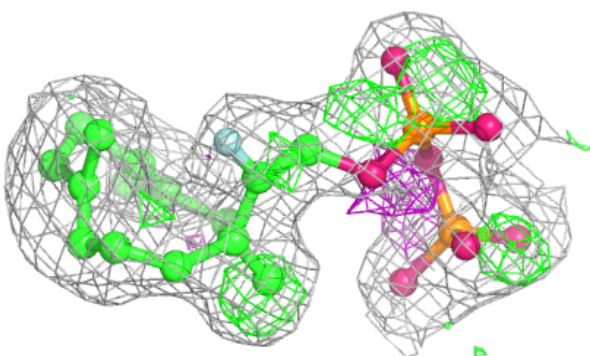
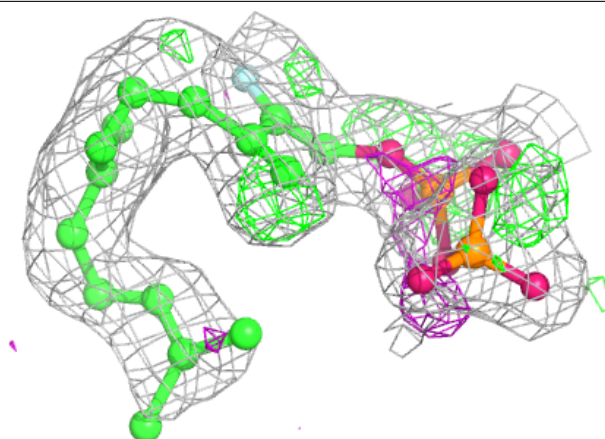
Electron density around FPF A 400:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FPF D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.